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FILE LAST UPDATED: 12 Sep 2006 (20060912/ED)

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L1 1 EP0474074/PN
(EP474074/PN)

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L1 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:214130 CAPLUS
DOCUMENT NUMBER: 116:214130
ENTRY DATE: Entered STN: 31 May 1992
TITLE: process for the preparation of dichlorobenzene (1,4-dichlorobenzene) by chlorination of benzene or chlorobenzene in the presence of Friedel-Crafts catalysts and N-[(perfluoroalkyl)carbonyl]phenothiazines
INVENTOR(S): Mais, Franz Josef; Fiege, Helmut
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Eur. Pat. Appl., 6 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
INT. PATENT CLASSIF.:
MAIN: C07C025-08
SECONDARY: C07C017-12
CLASSIFICATION: 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 35
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 474074	A1	19920311	EP 1991-114226	19910824 <--
EP 474074	B1	19940608		
R: BE, CH, DE, FR, GB, IT, LI				
DE 4028269	A1	19920312	DE 1990-4028269	19900906
JP 04305544	A2	19921028	JP 1991-244079	19910830
JP 2902171	B2	19990607		

PRIORITY APPLN. INFO.: DE 1990-4028269 A 19900906

PATENT CLASSIFICATION CODES:

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 474074	ICM	C07C025-08
	ICS	C07C017-12
	IPCI	C07C0025-08 [ICM,5]; C07C0025-00 [ICM,5,C*]; C07C0017-12 [ICS,5]; C07C0017-00 [ICS,5,C*]
	IPCR	C07C0017-00 [I,C*]; C07C0017-12 [I,A]
DE 4028269	IPCI	C07C0025-08 [ICM,5]; C07C0025-00 [ICM,5,C*]; C07C0017-12 [ICS,5]; C07C0017-00 [ICS,5,C*]; C07D0279-22 [ICS,5]; C07D0279-00 [ICS,5,C*]; B01J0027-128 [ICA,5]; B01J0027-06 [ICA,5,C*]; B01J0031-02 [ICA,5]
	IPCR	C07C0017-00 [I,C*]; C07C0017-12 [I,A]
JP 04305544	IPCI	C07C0025-08 [ICM,5]; C07C0025-00 [ICM,5,C*]; B01J0031-02 [ICS,5]; B01J0031-30 [ICS,5]; B01J0031-26 [ICS,5,C*]; C07C0017-12 [ICS,5]; C07C0017-00 [ICS,5,C*]; C07B0061-00 [ICA,5]

OTHER SOURCE(S): CASREACT 116:214130; MARPAT 116:214130

ABSTRACT:
A process for the preparation of dichlorobenzene comprises the chlorination of benzene or chlorobenzene in the presence of Friedel-Crafts catalysts and N-[(perfluoroalkyl)carbonyl]phenothiazines; dichlorobenzene thus prepared contains 1,4-dischlorobenzene as major fraction. Dichlorobenzene is a monomer for the preparation of polyphene sulfide and for the preparation of dyes (no data). A reactor was charged with benzene (100 parts by weight), FeCl3 (0.050 parts by weight), N-(trifluoroacetyl)phenothiazine (0.091 parts by weight), heated to 60° and chlorine (127 parts by weight) was passed through the mixture in 5 h. The product contained benzene (0.12% by gas chromatog.), chlorobenzene (42.90%), 1,2-dichlorobenzene (9.83%) 1,3-dichlorobenzene (0.08%), 1,4-dichlorobenzene (46.98%), and trichlorobenzenens (0.09%). The same process using N-(trichloroacetyl)phenothiazine gave a mixture containing 40.46% chlorobenzene and 40.08% 1,4-dichlorobenzene.

SUPPL. TERM: chlorination Friedel Crafts phenothiazine trifluoroacetyl benzene; regiochem Friedel Crafts fluoroacetylphenothiazine chlorination benzene

INDEX TERM: Friedel-Crafts reaction catalysts
(catalyst containing [(perfluoroalkyl)carbonyl]phenothiazine and, for regioselective dichlorination of benzene)

INDEX TERM: Regiochemistry
(of chlorination of benzene over iron trichloride/(trifluoroacetyl)phenothiazine)

INDEX TERM: Chlorination
(regioselective, of benzene over iron trichloride/(trifluoroacetyl)phenothiazine)

INDEX TERM: 7439-89-6, Iron, uses 7705-08-0, Iron trichloride, uses
ROLE: USES (Uses)
(catalyst containing [(perfluoroalkyl)carbonyl]phenothiazine and, for regioselective dichlorination of benzene)

INDEX TERM: 96124-86-6 100234-24-0, N-(Perfluorobutanoyl)phenothiazine 141135-78-6, N-(Perfluoropropanoyl)phenothiazine
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(catalyst containing iron trichloride and, for regioselective dichlorination of benzene)

INDEX TERM: 95-50-1P, 1,2-Dichlorobenzene
ROLE: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, as byproduct in regioselective dichlorination of benzene over Friedel-Crafts catalysts and (trifluoroacetyl)phenothiazine)

INDEX TERM: 92-84-2DP, Phenothiazine, N-[(perfluoroalkyl)carbonyl] derivs.

ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
INDEX TERM: 108-90-7P, Chlorobenzene, preparation
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by regioselective chlorination of benzene over Friedel-Crafts catalysts and (trifluoroacetyl)phenothiazine)
INDEX TERM: 106-46-7P, 1,4-Dichlorobenzene
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by regioselective dichlorination of benzene over Friedel-Crafts catalysts and (trifluoroacetyl)phenothiazine)
INDEX TERM: 71-43-2, Benzene, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(regioselective dichlorination of, over Friedel-Crafts catalysts and (trifluoroacetyl)phenothiazine)

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L2            1 WO9743041/PN

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L2   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        1997:752871  CAPLUS
DOCUMENT NUMBER:         128:36352
ENTRY DATE:              Entered STN:  03 Dec 1997
TITLE:                   Regioselective nuclear chlorination catalyst for
                         aromatic hydrocarbons and process for nuclear
                         chlorination
INVENTOR(S):             Mizusawa, Shigeru; Sunagawa, Kazuhiko; Hozumi, Toshio;
                         Nonaka, Tsugio; Matsuda, Toshiharu
PATENT ASSIGNEE(S):      Kureha Kagaku Kogyo K.K., Japan
SOURCE:                  PCT Int. Appl., 36 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                Japanese
INT. PATENT CLASSIF.:
            MAIN:        B01J031-02
CLASSIFICATION:          45-4 (Industrial Organic Chemicals, Leather, Fats, and
                         Waxes)
                         Section cross-reference(s): 25, 28, 67
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     --------------       ----   --------    --------------------    --------
     WO 9743041            A1    19971120    WO 1997-JP1609          19970514 <--
         W:  CN, JP, KR, SG, US, VN
         RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
     JP 3818321            B2    20060906    JP 1997-540732          19970514
PRIORITY APPLN. INFO.:                       JP 1996-145134      A   19960514
                                             WO 1997-JP1609      W   19970514
PATENT CLASSIFICATION CODES:
 PATENT NO.       CLASS  PATENT FAMILY CLASSIFICATION CODES
 --------------   -----  ----------------------------------------------
 WO 9743041       ICM    B01J031-02
                  IPCI   B01J0031-02 [ICM,6]
                  IPCR   B01J0031-02 [I,A]; B01J0031-02 [I,C*]; C07C0017-00
                         [I,C*]; C07C0017-12 [I,A]
 JP 3818321       IPCI   B01J0031-02 [I,A]; C07C0025-02 [I,A]; C07C0025-00
                         [I,C*]; C07C0017-12 [I,A]; C07C0017-00 [I,C*];
                         C07B0061-00 [I,A]
OTHER SOURCE(S):          MARPAT 128:36352
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ABSTRACT:
Ph 10H-phenothiazine-10-carboxylates or their (optionally halogenated or alkyl-, alkoxy-, nitro- or cyano-substituted) chlorinated derivs. and Lewis acids are useful as regioselective nuclear chlorination catalysts for aromatic hydrocarbons. The catalysts are advantageous in that the regioselectivity is not lowered even when the nuclear chlorination is conducted at a reaction temperature
exceeding 45° and that the regioselectivity is enhanced with an increasing degree of chlorination. Thus, chlorination of chlorobenzene (I) 246 in the presence of FeCl3 0.47 and Ph 10H-phenothiazine-10-carboxylate 4.7 g at 50° in the dark for 7 h gave a product mixture containing I 44.92, o-dichlorobenzene 7.34, m-dichlorobenzene 0.05, p-dichlorobenzene (II) 47.66 and trichlorobenzene 0.04% at II selectivity 87%.

SUPPL. TERM: chlorination selectivity phenothiazinecarboxylate catalyst; chlorobenzene chlorination selectivity catalyst; arom hydrocarbon chlorination selectivity catalyst; regioselectivity chlorination catalyst phenothiazinecarboxylate; Lewis acid catalyst arom hydrocarbon chlorination

INDEX TERM: Aromatic hydrocarbons, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Lewis acids and phenothiazinecarboxylate compds. as regioselective systems for chlorination of)

INDEX TERM: Chlorination catalysts
(Lewis acids and phenothiazinecarboxylate compds. as regioselective systems for chlorination of aromatic hydrocarbons)

INDEX TERM: Lewis acids
ROLE: CAT (Catalyst use); USES (Uses)
(nuclear chlorination catalysts; with phenothiazinecarboxylate compds. as regioselective systems for chlorination of aromatic hydrocarbons)

INDEX TERM: Regiochemistry
(of regioselective nuclear chlorination catalyst for aromatic hydrocarbons)

INDEX TERM: 71-43-2, Benzene, reactions 100-41-4, Ethylbenzene, reactions 106-42-3, p-Xylene, reactions 108-88-3, reactions 108-90-7, Chlorobenzene, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Lewis acids and phenothiazinecarboxylate compds. as regioselective systems for chlorination of)

INDEX TERM: 106-46-7P, p-Dichlorobenzene 622-98-0P, p-Chloroethylbenzene 1124-05-6P, 2,5-Dichloro-p-xylene 29797-40-8P, Dichlorotoluene
ROLE: IMF (Industrial manufacture); PREP (Preparation)
(Lewis acids and phenothiazinecarboxylate compds. as regioselective systems for chlorination of aromatic hydrocarbons in manufacture of)

INDEX TERM: 66721-07-1P, Phenyl 10H-phenothiazine-10-carboxylate 199526-64-2P, 4-Chlorophenyl 10H-phenothiazine-10-carboxylate 199526-65-3P 199526-66-4P, 4-Methoxyphenyl 10H-phenothiazine-10-carboxylate 199526-67-5P, Phenyl 2-chloro-10H-phenothiazine-10-carboxylate 199526-68-6P 199526-69-7P 199526-70-0P 199526-71-1P 199526-72-2P 199526-73-3P 199526-74-4P 199540-47-1P
ROLE: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(nuclear chlorination catalysts; with Lewis acids as regioselective systems for chlorination of aromatic hydrocarbons)

INDEX TERM: 7446-70-0, Aluminum chloride, uses 7705-08-0, Iron chloride (FeCl3), uses 174141-46-9, Antimony chloride
ROLE: CAT (Catalyst use); USES (Uses)

(nuclear chlorination catalysts; with phenothiazinecarboxylate compds. as regioselective systems for chlorination of aromatic hydrocarbons)

INDEX TERM: 92-39-7 92-84-2, 10H-Phenothiazine 98-88-4, Benzoyl chloride 100-07-2, p-Methoxybenzoyl chloride 122-01-0, 4-Chlorobenzoyl chloride 874-60-2, 4-Methylbenzoyl chloride
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reactant; reaction in manufacture of regioselective nuclear chlorination catalyst for aromatic hydrocarbons)